National Center for Computational Sciences (NCCS) Snapshot June 26, 2006

NCCS Systems

In preparation for the 50 TF upgrade, the operating system on the Cray XT3 (Jaguar) was upgraded to version 1.4.19 last week. This software release is required for the dual-core upgrade to be performed in July.

The week of June 26th, the operating system for the Cray XT3 development system (Rizzo) will also be upgraded to version 1.4.19 and the hardware will be upgraded to dual-core. These upgrades will allow the High-Performance Computing Operations and Scientific Computing Groups to begin testing applications with the dual-core system configuration.

NCCS Tours and Visits

On June 7–8, the DOE Advisory Committee had a productive 2 days at the NCCS. The sessions included an overview of computing and computational sciences at ORNL, presented by Thomas Zacharia, and a discussion on delivering the Leadership Computing Facility (LCF), presented by Arthur S. Bland. The Committee outlined several recommendations for continued improvement as the NCCS moves forward in the LCF Project. The sessions were viewed as being upbeat and positive, with commendations for the work that has been accomplished thus far.

On June 9, the NCCS hosted Clay Sell, the Deputy Secretary of Energy, during his first visit to ORNL in his current role. Dr. Sell's visit to ORNL presented the opportunity for Thomas Zacharia to introduce the LCF and the work that is being accomplished in the areas of climate, biology, fusion, and nuclear energy. The presentation also provided the background for discussions on the compelling need for big computers to play a leading role in DOE's Global Nuclear Energy Partnership (GNEP) Program (http://www.gnep.energy.gov/). The presentation by the NCCS allowed Dr. Sell to see and hear about the exciting and enabling work at ORNL that can directly contribute to the success of GNEP.

Science Highlights

Big machines enable big science at the NCCS. Over the past few weeks, researchers using the Cray XT3 and X1E have been able to achieve some of the largest fusion simulations to date. Using LCF allocations for Wei-li Lee's "Gyrokinetic Plasma Simulation" project and code developed by the research team, the researchers were able to run their gyrokinetic toroidal code (GTC) simulations on 4,800 processors (92% of Jaguar's 5,212-processor capacity) using 28 billion particles, making it one of the largest fusion simulations ever run.

Dr. Lee's project team is using the XT3 and X1E to simulate plasma turbulent fluctuations that cause particles and energy to travel from the center of the plasma and flow toward the edge. Turbulence causes the plasma to lose the heat that is essential to

maintaining the fusion reaction, so it must be understood and controlled to enable a fusion reactor to operate successfully. Reliable modeling of turbulence processes is an indispensable step toward formulation of control strategies. The allocation of time using NCCS resources makes it possible to address the convergence issues such as discrete particle noise and the production runs with real physics goals. Scott Klasky, project liaison, says that the team is already seeing results. Klasky says, “We’ve been able to see turbulent spreading, and we’ve been studying noise through ETG [electron-temperature-gradient] turbulence simulations, because we are able to put up a very large number of particles, which enables us to do convergence tests for noise studies.”